AANSS2024

ANBUG-AINSE Neutron Scattering Symposium

4 - 6 November 2024

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THE AUSTRALIAN INSTITUTE OF NUCLEAR SCIENCE AND ENGINEERING

Program

Day 1 | Monday, 4 November

08:30	**Registration Opens - AINSE Theatre**		
09:30	Welcome Address, Acknowledgement of Country & Housekeeping		
Session 1 - ANSTO Facility Updates | Karyn Wilde			
10:00	Update from the Australian Centre for Neutron Scattering	Jamie Schulz	#53
10:30	Deuterium labelling at the National Deuteration Facility: Updates on Demand and Supply	Tamim Darwish	#56
11:00	Morning Tea		
Session 2 - Magnetism and Condensed Matter | Kirrily Rule			
11:20	**Invited: Cycloidal spin textures in multiferroic BiFeO3 thin films probed by neutron diffraction**	**Daniel Sando**	**#19**
11:50	The anisotropic magnetism of the cobalt-doped rare earth iron garnet Lu3Fe4Co0.5Si0.5O12	Siobhan Tobin	#5
12:10	Investigating the perturbation to the spin ordering of the helimagnet Cu2OSeO3 upon doping	Samuel Yick	#9
12:30	Dynamic realignment of the antiferromagnetic structure of exchange-biased CoFe /MnPt	Danica Solina	#16
12:50	Lunch		
Session 3 - Magnetism and Condensed Matter | Dehong Yu			
13:50	**Plenary 1: Investigating quantum magnetism with neutron scattering**	**Bella Lake**	**#11**
14:50	Spin wave excitations and two sublattice interactions of 153EuMn2Ge2	Richard Mole	#37
15:10	Magnetic fans, propellers and twist structures: Micromagnetic simulations to describe polarised neutron reflectometry data	Karen Livesey	#38
15:30	Afternoon Tea		
15:50	Recent polarised neutron experiments at ACNS	Andrew Manning	#46
16:10	Short Break		
16:15	**Poster Slam | Chin-Wei Wang**		
18:15 - 20:30	**Poster/Networking Session in nandin**		

Program

Day 2 | Tuesday, 5 November

Session 4 - Manufacturing, Engineering & Industry | Ania Paradowska			
09:00	**Invited: ANSTO's Neutrons for Industry**	**Helen Qiu**	**#4**
09:30	Material Properties and Residual Stress Measurements in Additively Manufactured 316L stainless steel components	Markus Domogala	#33
09:50	Additive Friction Stir Deposition (AFSD) for High-Strength Aluminium Alloys	Vladislav Yakubov	#54
10:10	Morning Tea		
Session 5 - Biological Systems and Soft Matter | Erica Wanless			
10:30	**Invited: Using (U)SANS to study protein structures in complex mixture**	**Leonie van t'Hag**	**#12**
10:50	Water Dynamics in Australian Native Fruits as studied using Neutron Spectroscopy and Tomography	Paul Michalski	#17
11:10	Recent applications of neutron backscattering spectroscopy at ANSTO	Nicolas De Souza	#25
11:30	Specific Ion Effects on the Behaviour of a Pluronic Block Copolymer in the Bulk and at the Air/Water Interface	Grant Webber	#27
11:50	CLIC1 interaction with Model Membranes	Stephen Holt	#42
12:10	Lunch		
Session 6 - ANBUG 2024 Award Presentations | Chris Wensrich			
13:30	ANBUG Young Scientist Award		
13:50	ANBUG Neutron Award		
14:20	Afternoon Tea		
14:50	ANBUG Career Award		
15:50	ANBUG PhD Award		
16:10	ANBUG Annual General Meeting (AGM)		
17:20	Short Break		
17:30	**Plenary 2: Residual stress measurement and mitigation engineering**	**Philip Withers**	**#24**
18:30	**Pre-dinner Drinks & Networking**		
19:00	**Dinner at ANSTO Cafe**		

Program

Day 3 | Wednesday, 6 November

Session 7 | Chemistry and Crystallography - Helen Maynard Casely			
09:00	**Plenary 3: What a tame Platypus reveals about polymer brushes**	**Erica Wanless**	**#6**
10:00	Structural instability in BiVO4 under compression	Brendan Kennedy	#1
10:20	Modelling diffuse magnetic scattering in a “partial spin-liquid” kagomé compound	Chris Ling	#21
10:40	Automated Analysis of Neutron Reflection Data from a Lithium-Mediated Nitrogen Reduction Reaction Using Bayesian Evidence	Callum Weir-Lavelle	#28
11:00	Morning Tea		
Session 8 | Neutron Instruments & Techniques - Helen Qiu			
11:20	**Invited: ISIS Deuteration Facility**	**June McCorquodale**	**#18**
11:50	Rediscovery of lost art in Reflectometry - using Maximum Entropy to study ‘diffuse’ systems	Andrew Nelson	#15
12:10	Recent Scientific Highlights and Developments on the Spatz Neutron Reflectometer	Anton Le Brun	#26
12:30	Awards Presentation	Andrew Peele	
12:45	Lunch		
13:40	A Decade of Successful Operation and Future Perspectives	Dehong Yu	#32
14:00	Neutron reflectometry for in operando characterisation of the solid electrolyte interphase (SEI) in electrochemical lithium-mediated nitrogen reduction reactions (Li-NRR)	Rebecca Hodgetts	#44
14:20	AINSE	Michelle Durant	
14:45	Afternoon Tea		
Session 9 | Advanced functional materials & devices/Earth Environment & Cultural Heritage - Lu Jiang			
15:00	Studying device processing steps with neutron reflectometry: Examples from quantum technology	David Cortie	#41
15:20	Cultural Heritage research using neutron methods at ACNS	Filomena Salvemini	#48
15:40	Neutron Imaging for Palaeontology	Joseph Bevitt	#55
16:00	**Closing**		

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- ANBUG Women in Neutron Scattering Program
- Thanks to the ARC Georgina Sweet Australian Laureate Fellowship program
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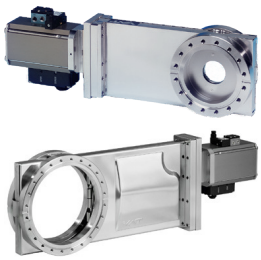

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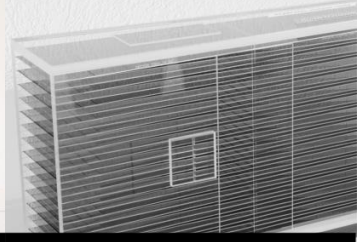

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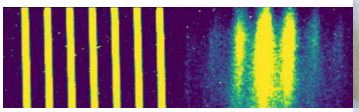

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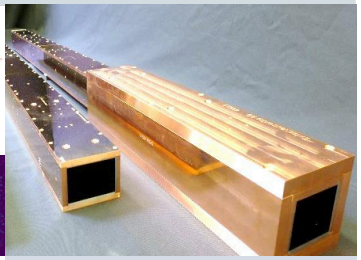

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Abstract Booklet

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Poster Presentations

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Poster Presentations

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57	Recent developments on Echidna	James Hester

Abstract #1

Structural instability in BiVO4 under compression

Bismuth Vanadate displays rich polymorphism, resulting in a complex structural phase diagram. Owing to its potential as a photocatalyst for hydrogen production understanding the factors that influence its structure are important. This presentation focus on variable pressure neutron diffraction studies that reveal BiVO4 undergoes an unusual increase in symmetry, from monoclinic to tetragonal, upon application of modest pressure. This correlates with a significant reduction in both the volume and distortion of the BiO8 polyhedra, consistent with pressure induced melting of the Bi 6s2 lone pair electrons. Conversely the VO4 tetrahedra are relatively incompressible. The behaviour of BiVO4 is compared to that of the isostructural oxide LaNbO4 that lacks lone pair electrons.

Author: KENNEDY, Brendan (The University of Sydney)

Abstract # 2

Modelling the magnetic exchange interactions relative to inelastic neutron scattering results in the quantum antiferromagnet atacamite

An experimental inelastic neutron scattering (INS) study on atacamite (Cu2Cl(OH)3) has been performed using Pelican to verify previous density-functional theory (DFT) calculations of its magnetic exchange interactions. INS reveals two dispersive spin wave modes along the H direction. Comparison with linear spin wave theory (LSWT) modelling indicates a frustrated zigzag-chain system along the crystallographic a direction. Additionally, the INS data reveals a spin wave gap along the H direction of at least 0.75 meV. LSWT modelling reveals that an additional perturbative term in the Hamiltonian is essential to reproducing the experimental spin wave gap. At first glance, the zigzag chain is not congruent with previous DFT results. We propose that the zigzag chain represents an effective model which is valid at low temperature, whereas the previously proposed sawtooth chain represents a Hamiltonian for atacamite whose characteristics are only present in a high-temperature regime.

Authors: **RULE, Kirrily (ANSTO),** ALLEN, Jackson (UOW); MOLE, Richard (ANSTO); LEWIS, Roger (University of Wollongong); Dr HEINZE, Leonie (Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ)); Prof. SUELLOW, Stefan (Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig)

Abstract # 3

The Martensitic Transformation in In-Tl Alloys Revisited

The traditional, "text-book" view [1] for the martensitic transformation in In-x at%Tl alloys, for 15.5 ≤ x ≤ 30.5, has been via a double shear such as: $(101)[\bar{1}01]$; $(011)[0\bar{1}1]$, on the basis of optical -microscopy observations [2] and measurements of the (c11 – c12)/2 elastic constant [3]. However, this model was called into question following measurements of the low -ζ, $[\zeta\zeta 0][\zeta\bar{\zeta}0]$ phonons, initially on the HB3 triple-axis spectrometer at the Oak Ridge National Laboratory [4], on the H7 spectrometer at Brookhaven National Laboratory [5] and more recently, at the Australian Centre for Neutron Scattering (ACNS), via Proposal DB6030, on the Sika cold-triple-axis spectrometer at the OPAL Research Reactor [6]. An alternative model for the formation of coherent nuclei and growth along conjugate {111} planes was once proposed by Geisler [7]. This model is consistent with some electron diffraction diffuse scattering data [8] as well as yielding identical x-ray pole figure results as those for the double-shear mechanism [7], where appropriate nuclei could be generated by $\langle 111\rangle\langle 11\bar{2}\rangle$ atomic displacements. To test such an idea we have measured the $[\zeta\zeta\zeta]$T phonon branch as a function of temperature, for a good quality, In-Tl crystal through ACNS proposal P7049, also on the Sika spectrometer. In addition, we are undertaking resonant ultrasonic spectroscopy (RUS) and transient grating spectroscopy (TGS) measurements on small crystals of In-Tl, which we have shown to exhibit the martensitic transformation, through a recent experiment on the Koala Neutron Laue Diffractometer at OPAL via ACNS proposal DB17489. The results of these various experiments will be presented and discussed, in relation to the traditional view for the transformation in In-Tl alloys.

References

[1] G.A. Chadwick. Metallography of Phase Transformations (Butterworths, London, 1972) p272.
[2] J.S. Bowles, C.S. Barrett and L. Guttman. "Crystallography of Cubic-tetragonal Transformation in the Indium-Thallium System", Trans. Metall. Soc. A.I.M.E. 188, 1478-1485 (1950).
[3] D.J. Gunton and G.A. Saunders. "The Elastic Behaviour of In-Tl Alloys in the Vicinity of the Martensitic Transformation". Solid State Commun. 14, 865-868 (1974).
[4] T.R. Finlayson and H.G. Smith. "Neutron Scattering Studies of Premartensitic Indium-Thallium Alloys", Metall. Trans. A 19A, 193-198 (1988).
[5] T.R. Finlayson, D. Donovan, J.Z. Larese and H.G. Smith. "Studies of Transverse Phonon Modes in Premartensitic Indium-Thallium Alloys". Materials Science Forum 27/28, 107-112 (1988).
[6] T.R. Finlayson, G.J. McIntyre and K.C. Rule. "The Martensitic Transformation in Indium-Thallium Alloys". Proceedings of the International Conference on Martensitic Transformations: (Chicago), eds. Aaron P. Stebner and Gregory B. Olsen (ISBN 9789-3-319-76968-4) (The Minerals, Metals & Materials Society, 2018) pp 291-297.
[7] A.H. Geisler. "Crystallography of Phase Transformations". Acta Metall. 1, 260-281 (1953).
[8] T.R. Finlayson, P. Goodman, A. Olsen, P. Norman and S.W. Wilkins. "An Electron Diffraction Study of a Pre-martensitic In-24 at.% Tl Alloy", Acta Cryst. B40, 555-560 (1984).

Authors: **Dr FINLAYSON, Trevor (University of Melbourne)**; MCINTYRE, Garry (ANSTO); RULE, Kirrily (ANSTO); Dr SEINER, Hanus (Czech Academy of Sciences)

Abstract # 4

ANSTO's Neutrons for Industry

Neutron scattering research at ANSTO covers various fields, including hydrogen, advanced material, food science, cultural heritage, mining, antibiotics, etc. The Australian Centre for Neutron Scattering (ACNS) utilises neutrons from Australia's multi-purpose research reactor, OPAL, to solve complex research and industrial problems for Australian and international users via merit-based access and user-pays programs. This presentation will introduce the industrial and commercial clients of ACNS, delineate the methods of access, and present case studies from several beamlines. The clientele includes consulting firms, research organizations, and industrial entities such as TOYOTA, CSIRO, and DMTC, spanning various sectors. Access is facilitated through different models depending on the stage of the product lifecycle and value chain of our partners. The first model is the merit program, designed for early-stage research with a willingness to publish results, often in collaboration with university partners. The second model is commercial, fee-for-service access, which offers tailored support from our experts and ensures confidentiality and intellectual property arrangements. Additionally, collaborative grants or tenders represent another access model for industry. The final model involves sovereign suppliers. The presentation will briefly overview the beamlines relevant to engineering applications, including their basic functions: Kowari, Dingo, Wombat/Echidna, Quokka/Bilby, Kookaburra, and Emu/Pelican, accompanied by illustrative case studies.

Authors: Dr QIU, Helen-Zhijun

Abstract # 5

The anisotropic magnetism of the cobalt-doped rare earth iron garnet Lu3Fe4Co0.5Si0.5O12

The rare earth iron garnets (IGs, REFe5O12, where RE is a rare earth) have been a source of scientific interest for decades due to their ferrimagnetic properties [1] and corresponding magnon dynamics [2]. The most famous rare earth IG, YIG, is the cornerstone of advances in spintronic technology, due to its exceptionally low magnon damping, microwave and magneto-optical properties [2]. Less well known are the magnetic excitations of other rare earth IGs, such as LuIG.

The rare earth IGs are described by space group *Ia3d*. The distribution of magnetic Fe ions among different sites leads to ferrimagnetism. Lu, being the smallest of the rare earths, is more likely to create antisite defects within the material. When combined with doping on the non-magnetic and magnetic sites, this leads to phenomena such as the inverse Faraday effect [3] and the spin Seebeck effect [4]. Lu3Fe4Co0.5Si0.5O12 is a specific example of doped LuIG with increased anisotropy due to the Co2+ substitution. Inherent in this large unit cell are frustrated exchange interactions. In a thin film sample this led to a magnetic phase transition at 200 K and an additional cluster spin glass phase below 190 K [5].

We have now studied Lu3Fe4Co0.5Si0.5O12 in the bulk, using a single crystal sample for inelastic neutron scattering on the PELICAN and TAIPAN instruments at ANSTO, and neutron diffraction on D10 at the ILL. Our results show a clear anisotropy gap and a smaller gap between the acoustic magnon modes compared to YbIG [6] and YIG [7], as well as magnetocrystalline anisotropy that is strongly temperature dependent. The key differences in the magnetic structure, spin wave spectra and exchange parameters will be discussed.

References

[1] R. Pauthenet. “Magnetic Properties of the Rare Earth Garnets”. Journal of Applied Physics 30.4, S290-S292 (1959).
[2] A. A. Serga, A. V. Chumak, and B. Hillebrands. “YIG magnonics”. Journal of Physics D: Applied Physics 43.26, 264002 (2010).
[3] A. H. M. Reid et al. “Optical Excitation of a Forbidden Magnetic Resonance Mode in a Doped Lutetium-Iron-Garnet Film via the Inverse Faraday Effect”. Physical Review Letters 105.10, 107402 (2010).
[4] R. Ramos et al. “Room temperature and low-field resonant enhancement of spin Seebeck effect inpartially compensated magnets”. Nature Communications 10.1, 5162 (2019).
[5] H. Yamahara, M. Seki, and H. Tabata. “High temperature spin cluster glass behavior in Co- and Si-substituted garnet ferrite thin films”. Journal of Magnetism and Magnetic Materials 501, 166437 (2020).
[6] V. Peçanha-Antonio et al. “Model for coupled 4f - 3d magnetic spectra: A neutron scattering study of the Yb-Fe hybridization in Yb3Fe5O12”. Physical Review B 105.10, 104422 (2022).
[7] A. J. Princep et al. “The full magnon spectrum of yttrium iron garnet”. npj Quantum Materials 2.1, 1-5 (2017).

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Abstract # 6

What a tame Platypus reveals about polymer brushes

The interfacial character of solids can be markedly altered by coating with a polymer brush to target a range of applications. Many techniques can reveal fundamental attributes of the brush such as thickness and solvation (ellipsometry), wettability (contact angle) or stiffness (quartz crystal microbalance with dissipation monitoring). However, only neutron reflectometry can reveal the internal brush nanostructure; the polymer volume fraction profile. We have used Platypus at ANSTO for the last decade to increase our understanding of brush structure in varied environments such as pH or ionic strength (for polyelectrolyte brushes [1,2]) or temperature (for thermoresponsive brushes [3,4]). Recently we have focused considerable attention on improving the modelling of the diffuse polymer brush volume fraction (VF) profiles.[5] Subtle features in the brush depth profile have traditionally challenged the interpretation of the acquired relatively featureless reflectivity profiles. Confidence in fitting has been increased by using a Bayesian statistical approach [6] and co-refinement of directly comparable ellipsometric data.[7] Using these approaches, subtle conformational changes in thermoresponsive polymer brush depth profiles have been revealed: these brushes undergo a well- to poorly-solvated phase transition over a given temperature range. These exemplar systems also readily reveal specific ion effects (character dependent on ion identity rather than solely ionic strength) when exposed to electrolytes from across the Hofmeister series.[4,8] Furthermore, nonmonotonic VF profiles have revealed (a) monomer enrichment near the substrate arising during copolymer brush synthesis,[9] or (b) ion binding to the brush.[10] Recent work has also deployed neutron reflectometry to probe brushes in nonaqueous solvents.[11] Finally, strong polyelectrolyte brushes are now helping us to probe the nature of the concentrated electrolyte phenomenon of underscreening which is not included in classical understanding of electrolytes yet is critical to interface optimisation in high salt environments such as batteries.[2]

References

[1]T. J. Murdoch et al., Macromolecules, 49, 9605 (2016).
DOI: 10.1021/acs.macromol.6b01897
[2]H. Robertson et al., Phys. Chem. Chem. Phys., 25, 24770 (2023).
DOI: 10.1039/D3CP02206D
[3]T.J. Murdoch et al., J. Colloid Interface Sci., 526, 429 (2018).
DOI: 10.1016/j.jcis.2018.04.086
[4]T.J. Murdoch et al., Macromolecules, 49, 6050 (2016).
DOI:10.1021/acs.macromol.6b01001
[5] H. Robertson et al., Adv. Colloid Interface Sci., 331, 103238, 1 (2024).
DOI: 10.1016/j.cis.2024.103238
[6] I. Gresham et al., J. Appl. Crystallogr., 54, 739 (2021). DOI: 10.1107/s160057672100251x
[7] H. Robertson et al., SoftwareX, 20 101225 (2022). DOI: 10.1016/j.softx.2022.101225
[8] T.J. Murdoch et al., Polymer, 138, 229 (2018). DOI: 10.1016/j.polymer.2018.01.053
[9] E.C. Johnson et al, Langmuir, 36, 12460 (2020). DOI: 10.1021/acs.langmuir.0c01502
[10] H. Robertson et al., J. Colloid Interface. Sci., 634, 983 (2023).
DOI: 10.1016/j.jcis.2022.12.114
[11] H. Robertson et al., Langmuir, 40, 335 (2024). DOI: 10.1021/acs.langmuir.3c02596

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Abstract # 7

Grafting siloxane-containing methacrylates from surfaces

Polymer brushes- densely packed polymer chains tethered by one end to an interface- are a useful tool to control the interfacial properties of a substrate. These properties can be fine-tuned by control of the chemistry of the constituent monomer, as well as the thickness and grafting density of the brush. One such example are brushes composed of poly(dimethyl siloxane) (PDMS). Owing to its siloxane (Si-O) backbone, PDMS exhibits various desirable properties, including high hydrophobicity and 'liquid-like' mobility. Surface-tethered PDMS chains have therefore demonstrated potential in a plethora of applications ranging from lubricating surfaces[1] to liquid-repellent coatings.[2]

Most existing techniques for the preparation of PDMS brushes do not control structural attributes such as the grafting density, film thickness and uniformity- properties which have been shown to have a large influence on the interfacial characteristics of the coating.[3]

To address this shortcoming, this study aims to synthesise and characterise polymer brushes based on structurally similar silicon methacrylate monomers including 3-[tris(trimethylsiloxy)silyl]propyl methacrylate (SiMA) and the bespoke 3-(3-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)propoxy)-2-hydroxypropyl methacrylate (SIGMA, provided by GEO Specialty Chemicals). These hydrophobic monomers resemble the structure of PDMS due to their pendant siloxane moieties and are amenable to synthesis via controlled radical polymerisation techniques. This allows brushes to be synthesised via a controlled "grafting-from" polymerisation, whereby polymer chains are grown directly from the surface, affording fine control over the grafting density, film thickness and polydispersity of the chains.

Initial characterisation experiments will probe the effect of solvent quality on the behaviour of the brushes via in situ ellipsometry, sliding contact angle measurements, quartz crystal microbalance with dissipation monitoring (QCM-D) and neutron reflectometry (NR). Subsequent investigations will explore potential applications of the novel polymer brushes as lubricating surfaces via atomic force microscopy friction measurements and combined rheometry-NR (rheo-NR). Initial synthetic results and in-situ swelling experiments will be presented.

References

[1] T. Wang, J. Yang, S. Chen, Y. Sun, X. Jia, H. Song, ACS Appl. Mater. Interfaces 2024, 16, 11134–11144.
[2] L. Wang, T. J. McCarthy, Angew. Chemie Int. Ed. 2016, 55, 244–248.
[3] I. J. Gresham, S. G. Lilley, A. R. J. Nelson, K. Koynov, C. Neto, Angew. Chemie - Int. Ed. 2023, 62, e202308008.

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Abstract # 8

High-throughput characterisation of salt-induced aggregation and re-entry of silica nanoparticles

Electrolytes form a critical component of many systems from biological processes to energy storage. The Debye Hückel Theory has been extensively used to describe simple aqueous electrolytes, yet many applications of electrolytes involve significantly more complex matrices containing salt mixtures, high concentrations, complex ions or other co-solutes. Hypersaline solutions is one area of complex electrolyte research which has received renewed interest due to the observation of underscreening behaviour across simulation,[1] surface force apparatus,[2] polymer brush [3] and colloidal stability experiments.[4] At sufficiently high concentration, there is a minimum in the electrostatic decay length beyond which the range of electrostatic interactions in solution exceeds those predicted by the classical Debye length.[5]

This electrolyte effect is dependent on both the ion identity and the electrolyte concentration, making systematic experimental characterisation using conventional approaches time consuming, costly and repetitive due to an extensive range of possible experimental conditions. Recently, automation has become an increasingly important tool in experimental design due to its capability to explore large sample spaces efficiently and the possibilities of integration of machine learning to facilitate autonomous research environments.[6]

We have used colloidal silica as a model system to develop a high-throughput approach to the preparation of colloidal samples and characterisation of their stability, enabling the characterisation of aggregation behaviour in more detail. Colloidal silica has long been known to aggregate in the presence of electrolyte, inducing changes in dispersion turbidity.[7] This turbidity change was measured via UV-visible spectroscopy on a microplate reader enabling fast characterisation of particle aggregation. Re-dispersion was observed in all electrolytes at high concentrations, and the aggregation behaviour differed depending on whether the particles were dispersed in the low or high concentration regime. The high data density achievable through this characterisation methodology enabled subsequent targeted condition selection for light scattering experiments and future neutron scattering work.

Authors: **DUNLOP, Geran (The University of Newcastle),** CRAIG, Vincent (Australian National University); PAGE, Alister (The University of Newcastle); WANLESS, Erica (The University of Newcastle); WEBBER, Grant (The University of Newcastle)

Abstract # 9

Investigating the perturbation to the spin ordering of the helimagnet Cu2OSeO3 upon doping

Magnetic Skyrmion lattices (SkL) are spin ordering which are topologically protected due to their quantised winding number. This, along with other helimagnetic orderings offer a plethora of fascinating phenomena for fundamental research and applications.[1] Cu2OSeO3 is an insulating multiferroic material that has shown to host SkL at specific conditions.[2] It possesses a magnetic structure with both ferromagnetic (FM) and antiferromagnetic (AFM) super exchange interactions being present and has a 3-up 1-down ferrimagnetic arrangement of Cu2+ ions.[3] The lack of inversion symmetry in the corner shared O-Cu4 tetrahedra lattice results in an appreciable DMI between Cu2+ sites; this competes with FM/AFM interactions leading to spin canting formation of helical/conical spin textures at different fields and temperature conditions.[2] Due to the absence of a crystallographic transformation throughout the temperature range alongside the formation of the magnetic phases, it has been commonly assumed that the structure plays a passive role in magnetic ordering.[3] Yet, published studies have challenged this assumption. The work by Wu et al. shows that internal expansion leads to a decrease in Tc for the helical to paramagnetic transition.[4] Furthermore, observation by Nishibori et al. shows that by applying a pressure, Tc increases as the unit cell volume contracts.[5]

In this work, we incorporated both magnetic and non-magnetic ions into the Cu2OSeO3 host. The inclusion of Te into the Se-sites and Co into the Cu-sites changed the crystal and magnetic structure, respectively. The skyrmion dynamics and spin interactions within these materials were then studied using synchrotron X-ray powder diffraction, neutron powder diffraction, small angle neutron scattering, and magnetometry. Using X-ray powder diffraction at the Australian synchrotron, we identify a structural anomaly where the Cu network distorts around the paramagnetic-helical ordering temperature. This alludes to the possibility that structure is also a contributing factor to the magnetic ordering of the material despite the lack of structural phase transition. Through neutron diffraction, we found that the magnetic response of the spin ordering is highly susceptible to chemical doping. This implies that the rigidity of the spin coupling might be affected by the both magnetic and non-magnetic dopants. Small angle neutron scattering of our samples confirmed the various helimagnetic ordering and their periodicity. Lastly, we also studied the magnetic interactions through magnetometry. These results give us insight as to the relationship between materials structure and magnetic ordering. This highlights the importance of the crystal structure and an avenue to design novel spintronic materials.

References

[1] S. Mühlbauer, et al., Science 323, 915 (2009).
[2] S. Seki, et al., Science 336, 198 (2012).
[3] J.-W. G. Bos, et al., Phys. Rev. B 78 (9), 094416 (2008).
[4] H. C. Wu, et al., J. Phys. D: Appl. Phys. 48, 475001 (2015).
[5] E. Nishibori, et al., Phy. Rev. B 102, 201106 (2020).

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Abstract # 11

Investigating quantum magnetism with neutron scattering

Quantum magnetism studies the behaviour of magnetic materials where quantum fluctuations suppress the well-known properties of conventional magnets such as long-range magnetic order and spin-wave excitations, and give rise to exotic behaviours. Strong quantum fluctuations are typically found in magnets with small magnetic moments such as spin-1/2, where the interactions between the moments are low-dimensional as for spin chains, or where the interactions compete with each other due to the geometry of the compound which is known as frustration. It is possible to make model materials engineered to exhibit specific quantum properties which can then be studied experimentally. The experimental technique of neutron scattering provides deep insights into their properties and allows quantitative comparison to theory. Examples of neutron scattering investigations will be given ranging from spin chains to materials with frustrated triangular and tetrahedra arrangements of magnetic moments. The quantum spin liquid state will also be discussed where extreme frustration completely suppresses magnetic order and the spins form a dynamic emergent state characterized by quantum entanglement.

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Abstract #12

Using (U)SANS to study protein structures in complex mixtures

Understanding protein-lipid-starch interactions and the resulting protein structures is crucial for evolving food technology, biological and biomedical applications of nanomaterials. Knowledge regarding the effect of the multiple components in the system on the nanostructure, within the context of the application, is needed. This will be presented in this talk for two examples 1) therapeutic peptide encapsulation in lipid self-assembly materials and 2) plant-based protein gels. 1) Small-angle neutron scattering and reflectometry with contrast-matched lipid phases in D2O has opened up the possibility to study individual components within a mixed lipid system. We have used these techniques to study biomimetic lipid cubic phases, to investigate encapsulation of viral fusion peptides for therapeutic applications [1,2]. The cytotoxicity assay showed that the toxicity toward HeLa cells was dramatically decreased when the cholesterol or peptide level in the nanoparticles increased. This suggests that the addition of cholesterol can improve the biocompatibility of the cubic phase nanoparticles, making them safer for use in biomedical applications. 2) Plant proteins like pulses have been garnering more attention as the plant protein market has been growing with the increasing demand for alternative protein sources. Plant proteins can be used to form texturized products, such as meat analogues, by going through gelation, which is most commonly induced with heating and cooling of the proteins. Pulse proteins have been proposed to be great candidates to produce meat analogues, however, the gelation mechanism that can exist between different plant sources is not fully understood. Pulse protein isolates from yellow pea, soy and faba bean that were extracted using different methods were used to understand how pH and salt content can affect protein solubility and protein composition, and how this in turn affects the gelation behavior. Ultra- Small-Angle Neutron Scattering using a Bonse-Hart diffractometer combined with time-of-flight SANS enabled investigating changes in the insoluble protein fraction (µm) and soluble globulin and albumin proteins (nm length scale) as well as the contribution of lipid/starch during gelation. By utilizing complementary techniques such as rotational rheology, dynamic light scattering, SEM and synchrotron radiation-circular dichroism spectroscopy as well as SAXS to link to protein folding, it was observed that the gelation mechanism depends on both the soluble protein and insoluble protein particles [3,4]. Despite exhibiting significantly different gelation pathways to form homogeneous or fractal gels, the gelation strength for the plant proteins were similar demonstrating the potential of fractal gels dominated by hydrophobic interactions.

References

[1] Milogrdozka et al., van 't Hag, ACS Nano, 2023, 17, 8598-8612
[2] Milogrdozka et al., van 't Hag, JCIS, 2024, 670, 563-575
[3] Tiong et al., van 't Hag, Food Structure, 2024, 40, 100374 4 Tiong et al., van 't Hag, Food Hydrocolloids, 2024, Under review

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Abstract #13

18 years of Wombat – the high intensity diffractometer at OPAL

Wombat is a high intensity neutron diffractometer located in the OPAL Neutron Guide Hall. It is primarily used as a high-speed powder diffractometer, but the high-performance area detector means that measurements have also expanded into texture characterisation and single-crystal measurements. Wombat is particularly optimized for the study of materials in situ and in operando, measurements which are often carried out in partnership with the ACNS sample environment team.

Over 18 years of operation, Wombat has been used to explore a broad range of materials, including: novel hydrogen-storage materials, negative-thermal-expansion materials, cryogenic minerals, piezoelectrics, high performance battery anodes and cathodes, high strength alloys, multiferroics, superconductors and novel magnetic materials. Our poster will highlight the capacity of the instrument, recent comprehensive characterisation measurements, and some recent results.

Authors: **MAYNARD-CASELY, Helen (ANSTO);** TOBIN, Siobhan; PETERSON, Vanessa (ANSTO); HESTER, James (ANSTO); WANG, Chin-Wei (National Synchrotron Radiation Research Center)

Abstract #14

A semiempirical Hartree-Fock and an analytical tight-binding approach to solid-state calculations for inelastic neutron scattering

The scattering function, S(Q,ω), representing the interaction between the incident neutron and the pseudopotential, representing an ensemble of atoms, may be determined in a variety of ways: Via classical force-field approaches, through electronic structure calculations, through analytical approaches and through a combination of one or both of the first two approaches and applying molecular dynamics to study systems under non-equilibrium conditions. Electronic structure calculations quickly become computationally intensive and opaque once more than several hundred atoms are involved in a cluster or unit cell that represents the system under investigation. Another completely different approach is to assume that every solid-state system under study is fundamentally different and solve the specific interaction equation analytically, using for example, a so-called tight-binding methodology.

In the case of neutron spectroscopy many systems investigated are dominated by hydrogen vibrations as the total scattering coefficient, total~82 Barn is approximately an order of magnitude larger than most total scattering coefficients from other elements. Scatter from hydrogen is mainly incoherent and therefore may be considered localised allowing potentially simple molecular models to be employed in the study of hydrogenous materials. Here a well-known Hartree-Fock semi-empirical calculation scheme is presented that is lightning fast for small molecules and adequate for large molecules, clusters, and dynamical studies.

Force constants are obtained by diagonalisation of the mass-weighted Hessian matrix to obtain the vibrational frequency for each mode assuming that each atomic-pair vibrates in a simple-harmonic fashion. The scattering function, S(Q,ω), is then calculated firstly assuming a one-atom oscillator, then secondly more thoroughly for each atom-pair vibration within the molecule/cluster. A number of benchmark molecules are reported on. Interestingly these rapid calculations give a very good estimation of the scattering function that can be used for initial peak identification and further analysis of the detailed electronic and vibrational structure.

Lastly the first results for an analytical approach are reported here. Rather than calculate an entire system, parts are estimated analytically, and vibrational spectra are very simply calculated.

Author: STAMPFL, Anton (ANSTO)

Abstract #15

Rediscovery of lost art in Reflectometry - using Maximum Entropy to study 'diffuse' systems

Many innovative data analysis approaches have been developed since the inception of the reflectometry technique. Unfortunately many of them have fallen out of active use due to the lack of software tools implementing those approaches. In this talk we'll explore some historical approaches used for the freeform modelling of 'diffuse' (continuously varying) scattering length density profiles, including Cubic-B-Splines and Maximum Entropy. We'll then explain why we've resurrected them, how they're particularly useful for modelling polymer brush systems, and their general applicability across a wide range of 'diffuse' systems where the structure may not be known a-priori.

Authors: **NELSON, Andrew (ANSTO);** PRESCOTT, Stuart (UNSW Chemical Engineering); WANLESS, Erica (The University of Newcastle); WEBBER, Grant (The University of Newcastle); GRESHAM, Isaac (The University of New South Wales); ROBERTSON, Hayden (University of Newcastle)

Abstract #16

Dynamic realignment of the antiferromagnetic structure of exchange-biased CoFe /MnPt

Neutron scattering studies were carried out on single crystal bilayers of exchange-biased MnPt(001)/CoFe grown epitaxially on MgO[001] using magnetron sputtering. Polarized neutron diffraction measurements taken around the hysteresis loop with sample aligned along the bias direction showed changing peak shape and width for the 101 reflections while the 100 reflection only showed weak intensity changes. This suggests a change in domain size in the out-of-plane direction while in-plane the domain size remains constant. The through-thickness anti-ferromagnetic structure of 100 nm thick MnPt films was successfully explained by a multi-domain model based on reorientation of the antiferromagnetic moments with a chiral structure. A model in which there is a partial twist at the turning points of the hysteresis loop with resulting relaxation and spin reorientation at saturation is consistent with the observations and provides an improved means to understand exchange-bias in thin films for use in future spintronic devices.

Authors: **Dr SOLINA, Danica (University of Technology Sydney); CORTIE, Michael (University of Technology Sydney)**; Dr SCHMIDT, Wolfgang (Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at ILL); Ms KRIEN, Cornelia (Leibniz-Institute for Solid State and Materials Research Dresden); Mr KALTOFEN, Rainer (Helmholtz-Zentrum- Dresden-Rossendorf, Intelligent Materials and Devices); RULE, Kirrily (ANSTO); Prof. SCHREYER, Andreas (Helmholtz-Zentrum Hereon)

Abstract #17

Water Dynamics in Australian Native Fruits as studied using Neutron Spectroscopy and Tomography

Food production is being challenged by population growth and increased drought. One way to manage these challenges may lie in using native fruits, which have unique sensory and nutritional properties. Local species are inherently well-adapted to the Australian climate, and local and global interest are emerging (Richmond et al. 2019). A barrier to the industry's growth, and an ongoing research question for fruit more generally, is understanding how to maximise the retention of nutritional and quality attributes over the course of preservation. This is particularly true for those processes which manipulate food moisture, prompting the need to also understand the behaviour of water in fruits as they are being processed. In this work, neutron spectroscopy and tomography are used in a novel application to study the dynamics of water in fruit, specifically in the context of native fruits.

Measuring the drying kinetics and water sorption isotherms of native fruits and how these change with processing has revealed increased water sorption compared to what has been observed for other foods such as apple. In this work, native fruits of varying moisture contents were subjected to neutron backscattering spectroscopy (de Souza et al. 2016) and neutron time-of-flight spectroscopy (Yu 2020). This revealed slower bound water and faster free water dynamics compared to similar foods reported elsewhere.

Neutron tomography has also revealed the local moisture transport in these fruits as they were processed under different conditions (Garbe et al. 2017). This was correlated to their differences in drying kinetics and subsequent quality. From the combination of these techniques, a link is suggested between their drought tolerance and the differences in water dynamics compared to other crops. This allows for improved understanding of the preservation of native fruits and offers insight into the unique water binding of these drought-tolerant crops.

References

Richmond, R., M. Bowyer and Q. Vuong (2019). Australian native fruits: Potential uses as functional food ingredients. Journal of Functional Foods 62: 103547.

de Souza, N. R., Klapproth, A., & Iles, G. N. (2016). EMU, the high resolution backscattering spectrometer at ANSTO. Paper presented at 13th AINSE-ANBUG Neutron Scattering Symposium, Sydney, NSW, Australia, 29-30 November 2016.

Yu, D. (2020). PELICAN –a time of flight cold neutron spectrometer – new capabilities. Neutron Scattering Symposium 2020 Abstract Booklet, Australia.

Garbe, U., Salvemini, F. & Paradowska, A. (2017). Neutron Imaging Applications on DINGO at OPAL. Paper presented at ICNS 2017 (International Conference on Neutron Scattering), Daejeon, South Korea, 9 to 13 July 2017. Retrieved from: http://www.icns2017.org/program.php

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Authors: **MICHALSKI, Paul (Monash University),** VAN 'T HAG, Leonie (Monash University); YU, Dehong (ANSTO), DE SOUZA, Nicolas (ANSTO - Australian Centre for Neutron Scattering); Dr GARBE, Ulf (ANSTO); Prof. RUDMAN, Murray (Monash University)

Abstract #18

ISIS Deuteration Facility

The ISIS Deuteration Facility was originally founded in 2008 as the Oxford Isotope Facility, under the leadership of Robert Thomas. Moving to Harwell in 2013, the facility is now established within ISIS to provide deuterated material to support the user programme.

As part of the wider support laboratories team, the Deuteration Facility is integral to advancing neutron scattering research, providing the scientific community with essential tools for exploring molecular structures and functions through deuteration, by enabling contrast variation and reducing coherence, thus offering deeper insights into materials at the atomic level. The facility has produced a broad spectrum of deuterated and hydrogenated chemicals, ranging from basic organic building blocks to complex molecules such as lipids, peptides, surfactants, ionic liquids, and pharmaceuticals. These compounds are critical for various scientific disciplines, including advanced materials science, life sciences, energy and soft matter.

This talk will present an overview of the facility at ISIS, including details on access and capabilities, along with recent research highlights and scientific collaborations

Authors: **Dr MCCORQUODALE, June (ISIS Neutron and Muon Source);** Dr YOUNGS, Sarah; Dr LI, Peixun; Dr TELLAM, James; Dr MA, Kun; Dr CHEN, Yao

Abstract #19

Cycloidal spin textures in multiferroic BiFeO3 thin films probed by neutron diffraction

The popular multiferroic BiFeO3 (BFO) is both ferroelectric and antiferromagnetic (AFM) at room temperature. A promising direction for this material is in the realm of antiferromagnetic spintronics – here AFMs are of particular interest as they respond faster than in ferromagnets. Moreover, BFO possesses magnon (spin wave) excitations in the GHz-THz range which could be harnessed in future low energy magnonics.

An important step towards harnessing magnonic excitations in BFO is to control the magnetic ordering, as this dictates the presence and energies of the magnon modes. The magnetic structure of BFO is characterized by a long-range spin cycloid which arises through magnetoelectric coupling of the ferroelectric polarization with the magnetic order. In epitaxial (single crystal) thin films of BFO, stimuli such as doping, strain, and substrate orientation can influence the cycloid properties, including its presence, propagation direction, and modulation period.[1]

In this presentation, I will give an insight into my work of the past ~8 years using neutron diffraction (ND) to understand cycloidal spin textures in epitaxial BFO films. I will start with an introduction to the cycloid and explain that while ND is the traditional probe for its characterisation, one should consider complementary measurements with new nanoscale probes. Next, through review of early ND experiments, I will describe the effect of biaxial epitaxial strain on cycloid stability, [2,3] and the influence of substrate crystallographic orientation and film thickness on the spin cycloid.[4,5]

I will conclude by describing our ongoing efforts to understand finer details of the cycloid: if and how the spin modulation forms in new low-symmetry triclinic phases of BFO,[8] and how the cycloid can be influenced by applied magnetic and electric fields. This detailed knowledge into spin textures in BFO will be important for engineering thin film systems useful for future magnonic architectures.

References

[1] S. R. Burns, O. Paull, J. Juraszek, V. Nagarajan, D. Sando, Advanced Materials 2020, 32, 2003711.
[2] D. Sando, A. Agbelele, D. Rahmedov, J. Liu, P. Rovillain, C. Toulouse, I. C. Infante, A. P. Pyatakov, S. Fusil, E. Jacquet, C. Carrétéro, C. Deranlot, S. Lisenkov, D. Wang, J.-M. M. Le Breton, M. Cazayous, A. Sacuto, J. Juraszek, A. K. Zvezdin, L. Bellaiche, B. Dkhil, A. Barthélémy, M. Bibes, Nat Mater 2013, 12, 641.
[3] X. Ke, P. P. Zhang, S. H. Baek, J. Zarestky, W. Tian, C. B. Eom, Phys Rev B 2010, 82, 134448.
[4] W. Ratcliff, D. Kan, W. Chen, S. Watson, S. Chi, R. Erwin, G. J. McIntyre, S. C. Capelli, I. Takeuchi, Adv Funct Mater 2011, 21, 1567.
[5] S. R. Burns, D. Sando, B. Xu, B. Dupé, L. Russell, G. Deng, R. Clements, O. H. C. Paull, J. Seidel, L. Bellaiche, N. Valanoor, C. Ulrich, NPJ Quantum Mater 2019, 4, 18.

Authors: SANDO, Daniel (University of Canterbury)

Abstract # 21

Modelling diffuse magnetic scattering in a “partial spin-liquid” kagomé compound

Fe4Si2Sn7O16 has a well-ordered complex composite layered structure that incorporates perfectly hexagonal kagomé lattices of high-spin Fe2+ (S = 2) cations. Below TN = 3.5 K it adopts a unique “striped” magnetic structure [1,2] that breaks hexagonal symmetry and leaves 1/3 of the spins geometrically frustrated in an apparent “partial spin-liquid” state down to at least 40 mK. Polarised neutron diffraction data collected on D7 at the ILL show persistent structured magnetic diffuse scattering below TN, consistent with short-range interactions among 1/3 of the HS Fe2+ sites. We have fit the diffuse magnetic scattering intensity with a Monte Carlo “big box” approach and a magnetic interaction approach. The determined signs and relative magnitudes of the spin exchange coupling are consistent between these two approaches and with the results of high-level DFT (meta-GGA SCAN functional) calculations. Our key result is that the first, second and third-nearest neighbour exchange interactions (J1, J2, J3) are all strongly antiferromagnetic. This may explain why Fe4Si2Sn7O16 does not adopt either of the conventional long-range-ordered kagomé states that preserve hexagonal symmetry: q = 0 “in-out”, in which third-nearest neighbours are ferromagnetic with respect to each other; or q = √3×√3 “spiral”, in which second-nearest neighbours are ferromagnetic with respect to each other. We propose that the partially ordered ground state of Fe4Si2Sn7O16, in which there are no strictly ferromagnetic relationships, is the best compromise when J1-3 are all strongly antiferromagnetic.

References

[1] CD Ling et al., Physical Review B 9 (2017) 180410
[2] S Dengre et al., Physical Review B 103 (2021) 064425

Authors: **LING, Chris (University of Sydney);** MARLTON, Frederick (University of Sydney); SOEHNEL, Tilo (The University of Auckland)

Abstract # 22

Mechanisms of molecular dynamics in anomalous thermal expansion of NaSICON-type ceramics

NaSICON-type materials (ceramic lattices of joined MO6 and PO4 polyhedra with interstitial alkali metals) are of interest due to their ability to have anisotropic metallic semi-conductivity due to delocalization of electrons along the octahedral chains.[1] “Filled” alkali metal containing NaSICONs have been shown to have positive thermal expansion, whereas some “empty” NaSICONs have been shown to have some anomalous thermal expansion.[2] Applications of these materials are due to their thermomechanical stability, with increased resistance to thermal shock. The temperature dependant properties have been studied for some empty NaSICON type materials[2, 3], but often there is no variable temperature neutron powder diffraction and Xray powder diffraction data. We aim to gather variable temperature neutron powder diffraction data along with X-ray powder diffraction data in combination with molecular dynamics simulations to characterise lattice distortion modes and the mechanism of anomalous thermal expansion of NaSICON-type ceramics.

References

[1] Leclaire, A.; Borel, M. M.; Grandin, A.; Raveau, B. A mixed-valence niobium phosphate with an empty nasicon structure: Nb2(PO4)3. Acta Crystallographica Section C Crystal Structure Communications 1989, 45 (5), 699-701. DOI: 10.1107/s0108270188013708.

[2] Woodcock, D. A.; Lightfoot, P.; Smith, R. I. Negative thermal expansion behaviour in the NZP phase NbTi(PO4)3. In Symposium on Solid-State Chemistry of Inorganic Materials II, Boston, Ma, Nov 30-Dec 04, 1998; Materials Research Society: WARRENDALE, 1999; Vol. 547, pp 191-196.

[3] Zhao, D.; Liang, P.; Su, L.; Chang, H.; Yan, S. Al0.5Nb1.5(PO4)3. Acta Crystallographica Section E Structure Reports Online 2011, 67 (3), i23-i23. DOI: 10.1107/s1600536811003886.

Authors: **CLARK, Kaylee (The University of Sydney)**, LING, Chris (University of Sydney); AVDEEV, Max (ANSTO, Australian Centre for Neutron Scattering)

Abstract # 24

Residual stress measurement and mitigation in engineering

Since they equilibrate internally, residual stresses are not outwardly apparent and so often combine with the applied stresses to cause unexpected failures. They are especially problematic because they are both hard to measure and their prediction requires a knowledge of the whole history of the part during manufacturing and in service, which is almost never available. Diffraction, and neutron diffraction in particular, is especially useful as diffraction is one of the few techniques able to measure the residual stress field in parts non-destructively. In this presentation I will discuss the challenges of making reliable residual stress measurements by diffraction and look at a number of examples where residual stresses are important discussing their measurement and implications. I will compare the merits of neutron diffraction compared to synchrotron diffraction. I will look at the measurement and management of stresses across a range of welding techniques. This work carries across to the emerging field of additive manufacturing, both powder and wire additive, where residual stresses can be significant and life limiting. I will also look at strategies for the minimisation of residual stress.

Authors: **Prof. WITHERS, Philip (Royce Institute, University of Manchester)**

Abstract # 25

Recent applications of neutron backscattering spectroscopy at ANSTO

The Emu μeV-resolution spectrometer is operated by ACNS at OPAL since 2016. The spectrometer enables measurements at correlation times from tens of ps to a few ns, as enabled by its Si(111) crystal backscattering setup and a Doppler drive offsetting incident energy by a few 10μeV. Current momentum transfer range is from 0.27 to 1.8 Å^-1.

Quasielastic neutron scattering (QENS) investigations in organic matter make up the bulk of applications on Emu, while nuclear hyperfine splitting and quantum rotational tunneling studies are also possible.

A few examples from biophysics and polymer science will be presented [1-4]. There is as well growing interest in understanding transport-related diffusion in ionic conductors and catalytic materials [5,6]. Further to fully-fledged QENS studies, elastic- and inelastic-fixed window scans add versatility to backscattering spectroscopy, as further illustrated by recent high impact studies [7,8].

References

[1] A Yamaguchi et al, “Quasielastic Neutron Scattering Study on Low-Hydrated Myoglobin inside Silica Nanopores”, Coll Surf A 698 (2024) 134559
[2] Y Ye et al, "Dynamic entity formed by protein and its hydration water", Phys Rev Research (2024) accepted
[3] KJ Bichler et al, “Position-Dependent Segmental Relaxation in Bottlebrush Polymers”, Macromolecules 57 (2024) 4729
[4] S Kim et al, “QENS study on local segmental dynamics of polyelectrolytes in complex coacervates”, Polymer 264 (2023) 125525
[5] EA Cheung et al, “Structure and dynamics in Mg2+-stabilized y-Na3PO4”, J Am Chem Soc 143 2021 17079
[6] V Skukauskas et al, “Probing the dynamics of methanol in copper-loaded zeolites via quasi-elastic and inelastic neutron scattering”, Front Chem Sci Eng (2024) in press
[7] T Kikuchi et al, “Detailed dynamical features of the slow hydration water in the vicinity of poly (ethylene oxide) chains”, J Chem Phys 160 (2024) 064902
[8] S Zheng et al, “Colossal electrocaloric effect in an interface-augmented ferroelectric polymer”, Science 282 (2023) 1020

Authors: DESOUZA, Nicolas (ANSTO - Australian Centre for Neutron Scattering); KLAP- PROTH, Alice (ANSTO)

Abstract # 26

Recent Scientific Highlights and Developments on the Spatz Neutron Reflectometer

The Spatz neutron reflectometer is a time-of-flight reflectometer with a vertical sample geometry. The reflectometer was originally the V18 BioRef reflectometer at the BER-II reactor in Berlin, Germany, and transferred to Australia. Spatz currently sits at the end of the CG2B cold guide and views the cold-neutron source of the 20 MW OPAL Research Reactor [1]. Spatz entered user service in late 2020 and since then the instrument has produced several high impact publications and implemented a program of upgrades. Due to the vertical sample geometry this means that sample environments that could not be used on the Platypus reflectometer due to its horizontal sample geometry can now be utilised for reflectometry. One such example of this is the use of the high temperature vacuum furnace to look at the formation of epitaxial graphene films on silicon carbide [2]. Other recent instrument upgrades include the installation of a vertical sample changer for automated sample changing and installation of high precision collimation slits. Upgrades for the near-future include new solid-liquid cells, and scoping for a new infra-red spectroscopy set-up. Recent scientific highlights include work investigating virus binding to cell membranes [3, 4], how changes in bacterial membrane composition relate to antibiotic resistance [5], determining the vertical morphology of different electron acceptor and donor blends in organic solar cells [6], characterisation of new biosensors [7], and re-entrant swelling of polyelectrolyte brushes [8]. This presentation will showcase some of the recent developments and highlights and outline future plans.

References

[1] A.P. Le Brun et al., J. Appl. Cryst. 56, 18 (2023)
[2] A. Pradeepkumar et al., RSC Adv. 14, 3232 (2024)
[3] Y. Correa et al., J. Colloid Interface Sci. 645, 627 (2023)
[4] I. Milogrodzka et al., J. Colloid Interface Sci. 670, 563 (2024)
[5] M.-L. Han et al. Cell Reports. 43, 114410 (2024)
[6] T.-Y. Huang et al., ACS Appl. Nano Mater. 7, 17588 (2024)
[7] U.M. Lankage et al., ACS Appl. Mater. Interfaces 15, 52237 (2023)
[8] H. Robertson et al., Phys. Chem. Chem. Phys. 25, 24770 (2023)

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Abstract # 27

Specific Ion Effects on the Behaviour of a Pluronic Block Copolymer in the Bulk and at the Air/Water Interface

Specific ion effects are phenomena dependent on ion identity, not merely its valence or concentration. Polymers are frequently used as exemplar systems to investigate specific ion effects,[1,2] where the behaviour of thermoresponsive polymers, such as polypropylene oxide (PPO), is modified by salt. The Pluronic series are block copolymers of hydrophilic poly(ethylene oxide) (PEO) and hydrophobic PPO, arranged in a PEO-PPO-PEO triblock structure; e.g. Pluronic F127.[3] Increasing temperature decreases PPO solubility leading to formation of micelles above the critical micelle concentration (CMC). The temperature at which micelles are formed is dependent on polymer concentration and added ion identity and concentration. The effect of an anion on physicochemical behaviour can be captured through the 'sho' (þ) parameter, an ion's interaction-site specific charge density.[4]

Here we will present data collected using newly designed and commissioned air-liquid trough sample environment for the PLATYPUS neutron reflectometer. An adsorbed layer of F127 at the aqueous solution/air interface was probed as a function of KF, KCl, KBr, KI and KSCN concentration at 22 °C and as a function of temperature for KF, KCl, KBr, KI, KSCN, LiCl, LiBr and LiI. Raw reflectivity data demonstrate subtle differences dependent on ion identity and temperature. Analysis using the refnx[5] package reveal changes in the layering of the PEO and PPO blocks in the adsorbed layer.

The bulk aqueous solution structure of F127 has also been characterised with dynamic light scattering and via small angle neutron scattering using QUOKKA. Potassium halides were again used to study impact of anion identity, concentration and temperature on F127 self-assembly and aggregate structure. This experiment further investigated F127 behaviour in complex solutions to investigate if the effective þ value determined in mixed electrolyte can be predicted assuming ideal mixing of the component ions.

References

[1] H. Robertson et al., J. Colloid Interface Sci. 586, 292–304 (2021).
[2] H. Robertson et al., Langmuir 40, 335-347 (2024).
[3] M. A. Abou-Shamat et al., Macromol. Chem. Phys., 1900173 (2019).
[4] K. P. Gregory et al., Chem. Sci. 12, 15007-15015 (2021).
[5] A. R. J. Nelson & S. W. Prescott, J. Appl. Crystallogr. 52, 193-200 (2019).

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Abstract # 28

Automated Analysis of Neutron Reflection Data from a Lithium-Mediated Nitrogen Reduction Reaction Using Bayesian Evidence

Ammonia has been identified as a carbon-free energy vector with the potential to fill some of the void to be left in the energy landscape as the planet decarbonises. To aid in the chances of an ammonia fuel being implemented, new and scalable production processes are being studied to enable its synthesis at off-grid renewable energy farms. Currently, the most viable method is the electrochemical-lithium-mediated nitrogen reduction reaction. The reaction works via lithium reduction at the surface of the electrode. The lithium then follows thermodynamically feasible reactions with dinitrogen to lithium nitride and with any labile protons in the system to produce ammonia. Despite this simple theory behind which the ammonia is formed the actual composition and morphology of the surface deposit undergoing the reaction is not known. The reaction's complexity is increased by the presence of a solid electrolyte interphase, produced by the decomposition of electrolyte species either electrochemically or upon interaction with reactive lithium species. The interphase is responsible for allowing uniform lithium plating and moderating in the influx of reactants at appropriate ratios to prevent undesirable hydrogen evolution.

This talk discusses the modelling of in-situ neutron reflectometry conducted on these reactive surfaces. The modelling of these data sets can be erroneously biased by restrictive and incorrectly deduced bounds especially when there is high uncertainty in the prior knowledge of surface morphology and composition. The method proposed here aims to avoid these pitfalls enabling automated modelling of the time-resolved data with data-led smoothing and evidence-based model selection.

Key points include:
- Automation for analysing large numbers of time-resolved datasets.
- Allowing the model to change between different time segments.
- Model selection using Bayes Factors.
- Smoothing infeasible outputs with data-driven bias.
- Dealing with multimodality in the posterior distribution.

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Abstract # 29

Revising Magnetic Features in a New 2D vdW Ferromagnet: Fe3GaTe2

Fe3GaTe2 is a 2D vdW layered material with an intrinsic ferromagnetism identified by above-room temperature Curie temperature (Tc) and a robust large perpendicular magnetic anisotropy (PMA). Previous studies have shown that 2D vdW ferromagnets are promising candidates for many magnetoelectronic devices and next-generation spintronic applications. However, these 2D materials must be stable at room temperature with long range magnetic order for the majority of spintronics applications [1-3]. Theoretically, long-range ferromagnetism hardly exists in 2D materials because of thermal fluctuation and reduced spatial dimensionality but long-range order can be stabilised by the anisotropy-driven spin-wave excitation gap. Despite this, no intrinsic 2D vdW ferromagnetic crystals such as CrI3, Cr2Ge2Te6 and Fe3GeTe2 have ordered magnetic states at room temperature. To date, the 2D vdW ferromagnet with the highest Curie temperature is Fe3GaTe2, which has Tc (~350-380K), a high saturation magnetic moment (40.11 emu/g) and large PMA energy density (~4.79 X 105J/m3) with hexagonal structure of space group P63/mmc (a = b = 3.9860 Å, c = 16.2290 Å, α = β = 90°, γ = 120°) [2].

The study aims to revise magnetic properties of Fe3GaTe2 by investigating its magnetic structure. Initial measurements of polycrystalline samples, obtained by manual grinding of bulk crystals, using neutron powder diffraction (wavelength 2.41Å, Echidna diffractometer at ACNS), revealed a sharp peak near q=0.25Å-1 at 4K, which transitioned into a broad peak at 400K. However, Small Angle Neutron Scattering with Bilby indicated that this peak was an artifact of measurement limitations rather than a genuine magnetic signal. Further investigations using the Thermal Triple Axis Spectrometer with Taipan (wavelength of 2.345 Å) revealed at least one new magnetic peak arising below 100K. To identify different magnetic phases more precisely, single Fe3GaTe2 crystal will be analysed using neutron single crystal Laue diffractometer with Koala later this year.

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Abstract # 30

Determining the micellar composition of sulfobetaine surfactants through small-angle neutron scattering and molecular dynamics simulations

Sulfobetaines are zwitterionic surfactants with peculiar properties such as high foam stability, temperature resistance and salt tolerance (SiTu et al., 2017). Sulfobetaines are widely used in body care products and kitchen detergents. Despite their widespread use, micelle self-assembly and packing are not explored. In this work, we study hydroxyl sultaines to develop high-performance and environmentally friendly fluorine-free firefighting foam due to their suitability to withstand harsh conditions. This study combines small-angle neutron scattering (SANS) and molecular dynamics (MD) simulations to investigate the micellar architecture of sulfobetaine surfactants.

SANS experiments were conducted for three lauramidopropyl-derived zwitterionic surfactants in different temperatures and concentrations to probe the micellar structure in solution. Analysis revealed the presence of ellipsoidal micelle with a well-defined core-shell morphology. This allowed the determination of optimal headgroup area, volume of core, aggregation number and packing parameter. These experimental findings are complemented by atomistic MD simulations. We made the models of preformed micelles of various sizes and subjected the simulation trajectories to analyse the micelle size, eccentricity, solvent-accessible surface area and self-diffusion. Simulated radii and eccentricity of the micelles showed the fluctuations in the major and minor of the ellipsoid's axes confirming the ellipsoidal model fitted by SANS. Exploring the internal composition of micelle gives fair knowledge about surfactant packing in solution and this knowledge will be used to make better firefighting agents out of sulfobetaine precursors.

References

SiTu, W.X., Lu, H.M., Ruan, C.Y., Zhang, L., Zhu, Y., & Zhang, L. (2017). Effect of polymer on dynamic interfacial tensions of sulfobetaine solutions. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 533, 231-240. https://doi.org/https://doi.org/10.1016/j.colsurfa.2017.09.006

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Abstract # 31

Emu, the high-resolution neutron spectrometer: Its successes and challenges

Emu is the high-resolution neutron spectrometer installed at the OPAL reactor, ANSTO.
It is well suited to characterizing diffusion and tunneling processes, such as occurring in e.g. polymer chains, membranes, proteins, molecular crystals, with relaxation times from a few 10 ps to over 1 ns due to Emu's high energy transfer resolution (1 μeV FWHM) and accessible ±31 μeV energy transfer range. The spectral resolution is achieved by neutron backscattering from Si (111) crystals on the primary and secondary flight paths, allowing up to 1.95 Å-1 momentum transfer range [1]. Experiments are merit-based accessed and can be performed over temperatures ranging from 50 mK up to 800 K. Other sample environments such as pressure, magnetic fields, controlled gas delivery, etc. are also available.

The Emu spectrometer has been operational for seven years, effectively servicing both Australian and global users. Through continuous quality enhancement efforts, Emu now yields 4-5 high-impact papers annually. In this presentation, we will discuss instrumental challenges and successes encountered over its operational lifespan. Noteworthy studies from the Australian backscattering spectrometer, particularly in the fields of polymer science and biophysics, will be emphasized.

References

[1] N. R. de Souza et al., Neutron News, 27, 20 (2016).

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Abstract # 32

PELICAN – A Decade of Successful Operation and Future Perspectives

The time-of-flight direct-geometry neutron spectrometer, Pelican [1,2], has been serving the scientific community for 10 years, delivering exceptional scientific outcomes. Nearly 100 publications have emerged from research spanning quantum magnetism, energy materials, and liquid dynamics in biological and metallic systems. Notably, over a quarter of these publications have appeared in high-impact journals (Impact Factor > 8), including Nature, Nature Materials, Nature Physics, Physical Review Letters, Chemistry of Materials, and others. Pelican has become one of the most in-demand instruments at ACNS, with an oversubscription factor exceeding 3 in recent years. A strong national and international user community has also been established, driven in part by the instrument's reliability, which consistently surpasses 98% uptime.

A suite of advanced sample environment equipment—including ultralow temperatures, high magnetic fields, high temperatures, high pressures, and electric fields—has been developed, significantly enhancing the instrument's capabilities. Over the past decade, numerous students and early-career scientists have received valuable training on Pelican, advancing their scientific careers.

These accomplishments over the past decade would not have been possible without the dedication of the instrument team, the strong support from the operational staff, and the scientific contributions of an outstanding user community.

In this presentation, I will reflect on Pelican's 10 years of service to the scientific community, discussing our successes, areas for improvement, and future directions, both in terms of scientific impact and instrumentation development.

References

[1] D. H. Yu, R. A. Mole, T. Noakes, S. Kennedy and R. Robinson, J. Phys. Soc. Jpn., 82, SA027 (2013).
[2] D. H. Yu, R. A. Mole, and G. J. Kearley, EPJ Web of Conferences 83, Art. No. 03019 (2015)

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Abstract # 33

Material Properties and Residual Stress Measurements in Additively Manufactured 316L stainless steel components

Additive manufacturing techniques, including Wire-Arc Additive Manufacturing (WAAM), present new opportunities to reduce manufacturing costs and minimise waste in diverse industries like aerospace, nuclear and civil engineering. WAAM is favoured over other metal additive manufacturing methods for this sector due to its high deposition rates and ability to produce large, complex structures without build environment limitations. Moreover, WAAM enables the creation of unique and customized geometries for structural parts, offering engineers unprecedented design flexibility and the potential for enhanced structural and corrosion-resistant properties - distinct advantages of additive manufacturing.

Currently, the broad industrial implementation of WAAM is held back by a lack of extensive systematic research and standardization. One of the major challenges is the limited understanding of residual stress distribution within built components, both in experimental and simulation settings. Given the expectation of a strong texture with large grain sizes, this study investigates the residual stress state using neutron diffraction and the contour method in 316L stainless steel components. This paper focuses on understanding the role of the material's texture and the residual stress distribution within large-scale WAAM components.

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Abstract # 34

Pelican focussing guide project

The Pelican spectrometer has been in operation at the Australian Centre for Neutron Scattering (ACNS) for the past decade. This versatile instrument is designed for a wide range of measurements on powders, single crystals, and liquids, offering broad wavelength and resolution capabilities suitable for various scientific applications. Inelastic neutron scattering (INS) experiments often require high neutron fluxes due to the inherently weak intensity of scattered neutrons. This requirement limits the minimum sample size for neutron scattering measurements and poses challenges for experiments involving high pressure, deuteration, and single crystal growth.

To address these challenges, the Pelican team has designed, procured, and installed a supermirror focusing neutron guide. This upgrade has been optimized to significantly enhance the neutron flux at the sample position, increasing it by an order of magnitude at a 1 cm × 1 cm spot. While this improvement boosts the flux at the sample, it does lead to an increase in beam divergence and thus a reduction in Q resolution. The guide system is installed on a pair of translatable stages so they can be moved into the beam as required.

In this presentation, I will discuss the scientific rationale behind this major upgrade, provide details on the design and installation of the supermirror focusing neutron guide, and share preliminary results from this enhancement to the Pelican spectrometer.

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Abstract # 35

Thermal-Neutron Triple-axis Spectrometer Taipan and Its Future Upgrade at ANSTO

Taipan is a high-flux thermal-neutron triple-axis spectrometer with a traditional single-detector design. Taipan has been the power horse for thermal neutron inelastic neutron scattering experiments in Australian Centre for Neutron Scattering (ACNS) at Australian Nuclear Science and Technology Organisation (ANSTO) for the last ten years,[1] generating numerous beautiful scientific highlights, ranging from phonon dispersion in thermoelectric materials[2], to spin-wave spectrum in multiferroics[3], and to magnetic diffractions in 100nm BiFeO3 thin films[4,5]. Following the current trend for the neuron instrumentation worldwide,[6] it is interesting to consider a future upgrade of Taipan to increase its data-acquisition efficiency with a multi-analyser design. In this work, a flexible multi-analyser design is proposed for Taipan, and the advantages of such an upgrade are discussed via simulations. In contrast to the current Taipan with the single-detector design, the multi-analyser Taipan with 21 analyser channels will be able to simultaneously collect 21 different Q positions at the same energy transfer, providing at least one order of magnitude faster in data-acquisition rate. The splitting angle of the neighbouring channels is flexible and able to change from 1.5˚ to 2.5˚. The energy and Q resolutions of all the channels are simulated at two different final energy configurations,[7] namely, Ef = 8.07 meV and 14.87 meV, to determine the optimized splitting angle for the most efficient data acquisition. The simulated results demonstrate that the data-acquisition efficiency on Taipan can be enhanced to one order of magnitude higher by implementing the new multi-analyser design. Different splitting angles are suitable for different types of scans depending on the purpose of the experiments. According to simulation, high performances are expected from the upgraded multi-analyser Taipan, as demonstrated on the cold-neutron triple-axis spectrometer Sika.[8,9]

References

[1]. S. A. Danilkin et al., Neutron News 20, 37 (2009)
[2]. J. Qi et al., Nat. Commun. 11, 5197 (2020)
[3]. G. Deng et al., Phys. Rev. B 97, 085154 (2018)
[4]. J. Bertinshaw et al. Nat. Commun. 7, 12664 (2016)
[5]. S. R. Burns et al., npj Quantum Mater. 4, 18 (2019)
[6]. M. Kempa et al., Physica B 385–386, P1080-1082 (2006)
[7]. J. Šaroun and J. Kulda, Physica B 234–236, P1102-1104 (1997)
[8]. C.M. Wu, G. Deng, et al. J Instr. 11, P10009 (2016)
[9]. G. Deng and G. J. McIntyre, Nuclear Instr. Methods in Phys. Res. A 959, P163509 (2020)

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Abstract # 36

Optimizing Lipid Cubosomes for Alzheimer's Drug Delivery: Impact of Lipid Composition and Stabilizers

The increasing prevalence of age-related central nervous system disorders, including Alzheimer's disease (AD) which is the most common form of dementia, is not effectively addressed by existing treatments, which fail to significantly alter the neurodegenerative progression of AD. Lipid nanoparticles, including cubosomes, are a promising approach to enhance the delivery of bioactives to the brain through improved drug bioavailability and specific targeted drug delivery while minimizing adverse effects [1–4].

In this study, monoolein-based cubosome formulations were assessed as delivery vehicles for therapeutics used to treat AD. A polytherapy approach was used, including the clinically used AD drugs galantamine and memantine in combination with neuroprotective polyphenols. The drug and polyphenolic compounds were loaded in cubosomes of various lipid compositions to form biomimetic cubic phases. Cubosomes were characterized using small angle X-ray scattering (BioSAXS beamline), cryo-TEM, dynamic light scattering and encapsulation efficiency. Small angle neutron scattering combined with selective contrast matching was further used to assess the location of the therapeutics within the cubic nanostructure.

The addition of the AD drug galantamine and memantine preserved the internal cubic phase nanostructure, while the polyphenols induced a concentration dependent phase transition or phase separation. Stabilization of the cubosomes was successfully achieved using a range of different stabilizers enhancing brain delivery while minimizing cytotoxicity. Neutron scattering studies of memantine suggested homogeneous encapsulation of the three-dimensional structure in the lipid bicontinuous cubic phase. Overall, the high-throughput studies successfully achieved biomimetic cubic phases, suggesting their potential to deliver AD drugs and neuroprotective compounds to the brain.

References

[1] Zha, S. et al. ACS Nano 18, 1820–1845 (2024)
[2] Azhari, H. et al. Int J Pharm 600, (2021)
[3] Mohammad, Y. et al. J Colloid Interface Sci 605, 146–154 (2022)
[4] Cai, X. et al. Advanced Functional Materials (2024)

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Abstract # 37

Spin wave excitations and two sublattice interactions of 153EuMn2Ge2

The magnetic properties of the ThCr2Si2 type rare earth intermetallics have been shown to display a diverse range of physical properties including superconducting and magnetocaloric behaviour. The europium-based intermetallics are of particular scientific interest due to their intermediate valence, as highlighted by the series EuMn2Ge2 and EuMn2Si2 which demonstrate thermally driven valence transitions3 with EuMn2Ge2 of particular interest due to the intermediate valence and thermally driven valence transition. While neutron diffraction has demonstrated that the Mn sublattice orders at 667(9) K, more recent work has demonstrated that the Eu undergoes a transition to magnetic long range order at 10 K.

Here we report the inelastic neutron scattering investigation of the rare earth intermetallic EuMn2Ge2 carried out at Pelican, ACNS, ANSTO over the temperature range ~1.5 K – 20 K. The spectrum shows a complex temperature dependence with a different spectrum observed at 7 K and above this temperature, despite being in the same ordered phase. These observations have been modelled using linear spin wave theory (LSWT), this has allowed us to parametrise the exchange Hamiltonian and rationalise the observation of a spin gap.

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Abstract # 38

Magnetic fans, propellers and twist structures: Micromagnetic simulations to describe polarised neutron reflectometry data

Can simple mechanical rotation in an applied field be used as a tool to twist the spin-structure of a magnet at nanometre scales?

Here we present a simple 1D micromagnetic simulator (microM-ref1D) which is integrated with the Ref1D software for polarised neutron reflectometry to provide self-consistent fitting to magnetic thin film data in different field rotations. This is parametrised in terms of the fundamental exchange interactions, interface exchange terms, and anisotropy of the film layers.

Using this new software approach, we show that the exchange interaction at a ferromagnetic/antiferromagnet interface, when combined with a mechanical rotation of the film in an applied field, can be used to manipulate magnetisation at the nanoscale, to wind a variety of distinctive 1D magnetic structures: exchange springs, fans, propellers and solitons. Each of these structures can be identified by its unique finger print in the Q-dependent neutron spin flip signal of the reflection pattern. The winding angles are determined, primarily, by the exchange stiffness term which is related to the exchange interaction.

A proof-of-concept experiment using the Platypus polarised reflectometer at the ACNS was conducted to explore the magnetic winding in the well-characterised Ni80Fe20/α-Fe2O3 thin film system[1,2]. After field-cooling and rotation, the presence of a non-collinear component in the spin structure was detected using neutron spin flip analysis. We rule out slow relaxation effects using time-resolved rebinning of the time-of-flight data. We find we can describe the data well using the 1D micromagnetic model for the twist,[3] with the caveat that one additional parameter is needed to describe domain formation. These promising results imply that the mechanical rotation method has the potential to generate numerous stable and exotic non-collinear magnetic structures. Furthermore, the 1D micromagnetic simulation approach is a general strategy that can be widely applied in polarised neutron reflectometry fitting to constrain complex models. The benefit using this physical model, is that it also simultaneously describes or predicts other testable magnetic properties such as the coercive field, magnetization, Curie temperature and ferromagnetic resonance frequency to provide a holistic description of the magnet.

This research was supported by an IEEE Magnetics Society Education Seed Grant awarded to G. Causer and D. Cortie

References

[1] D. L. Cortie et al. Phys. Rev. B 86, 054408 (2012).
[2] G. L Cortie, D.L Cortie et al, Japanese J. Appl. Phys. 59 (SA), SAAC03 (2019).
[3] B. McGrath, K. L. Livesey & R. E. Camley, submitted (2024).

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Abstract # 40

Characterising the SEI of lithium-mediated electrochemical nitrogen reduction via in operando X-Ray Radiography

To combat climate change, many industries are trying to reduce their greenhouse gas emissions via clean fuels such as hydrogen. However, hydrogen gas is not energy dense, so finding efficient methods of storing hydrogen is critical. Nitrogen reduction to ammonia is a promising form of hydrogen storage because of ammonia's increased relative energy density and pre-existing transport infrastructure. Due to the energy-intensive nature of the traditional Haber-Bosch process to produce ammonia, alternatives like electrochemical nitrogen reduction are being explored. Reduction in organic media via a lithium mediator (LiNRR) has been shown to be a viable alternative process, with some systems optimised for high efficiency, and others for sustained production.[1,2]

LiNRR utilises much of the same electrolytes as Li batteries, so understanding the solid electrolyte interphase (SEI) is key to optimising conditions for high faradaic efficiency and ammonia yield. To better understand SEI formation, in operando X-Ray radiography was done on electrochemical LiNRR experiments with select conditions. Subsequent image processing using ImageJ and Noise2Void (N2V)[3] was able to give us useful information on SEI growth and gas evolution rates as the experiments progressed. Radiography images were then corroborated with ex situ SEM-EDX maps. Future experiments using other types of imaging, such as neutron radiography, may provide even greater insight on how the SEI builds over time.

References

[1] Du, H.-L.; Chatti, M.; Hodgetts, R. Y.; Cherepanov, P. V.; Nguyen, C. K.; Matuszek, K.; MacFarlane, D. R.; Simonov, A. N. Electroreduction of Nitrogen with Almost 100% Current-to-Ammonia Efficiency. Nature 2022, 609 (7928), 722–727. https://doi.org/10.1038/s41586-022-05108-y.
[2] Li, S.; Zhou, Y.; Fu, X.; Pedersen, J. B.; Saccoccio, M.; Andersen, S. Z.; Enemark-Rasmussen, K.; Kempen, P. J.; Damsgaard, C. D.; Xu, A.; Sažinas, R.; Mygind, J. B. V.; Deissler, N. H.; Kibsgaard, J.; Vesborg, P. C. K.; Nørskov, J. K.; Chorkendorff, I. Long-Term Continuous Ammonia Electrosynthesis. Nature 2024, 629 (8010), 92–97. https://doi.org/10.1038/s41586-024-07276-5.
[3] Krull, A.; Buchholz, T.-O.; Jug, F. Noise2Void - Learning Denoising from Single Noisy Images. arXiv April 5, 2019. https://doi.org/10.48550/arXiv.1811.10980.

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Abstract # 41

Studying device processing steps with neutron reflectometry: Examples from quantum technology

Nanoscale thin films and surface coatings play an integral role in advanced devices for electronics, energy, spintronics and quantum technology. In order to prepare devices, the materials are typically subjected to a wide range of device processing conditions. This may include dozens of steps including film deposition, gas exposure, heat treatment, photolithography, liquid etching and ion beam implantation. Each individual step can introduce chemical and structural modifications, and unwanted defects, so it is essential to track and characterise the film between steps, and where possible, deploy in-situ techniques to optimise the processing in real-time.

Here I will give an overview of the neutron reflectometry beamlines at ANSTO, including the new technical capabilities added since 2023, highlighting methods for studying electronic device processing steps. The capabilities include:

- Rapid vacuum annealing to temperatures of 1100 °C whilst measuring neutron reflection;
- Parallel beam optic diffraction experiments to enable simultaneous reflectometry and grazing incidence diffraction studies on Spatz for nanometer and angstrom-scale information on surface regions;
- In-situ four-probe resistivity measurements during heating or hydrogen gas treatments;
- Cryogenic magnetic field experiments to measure polarised neutron reflectometry on spintronic or superconducting layers from 5 K to 300 K, in 1 Tesla under in-plane field rotations up to 270 degrees;
- Off-specular and half-polarised reflectometry of microscale lithographic patterns (5-50 µm);
- Complementary ion implantation experiments using a MEVVA ion source and isotopically-resolved (mass separated) low energy implanter;
- Complementary susceptibility, quantum oscillations, magnetoresistance, resistivity and Hall Effect measurements ;
- Complementary X-ray reflectometry, grazing incidence diffraction and ellipsometry measurements;

To show the capabilities in action, I'll highlight collaborative work applied to quantum technology. This includes growth of novel superconducting films, in-situ growth of graphene-on-SiC, studying ion implantation in topological insulator materials and metal-polymer hybrid structures [1-4]. If time permits, I will discuss several upcoming and optional developments with the goal of getting feedback from the user community on:

- A vacuum suitcase for transporting air-sensitive samples between processing steps;
- Thin film deposition system integrated with vacuum suitcase for adjusting isotopic contrast;
- 3He fully enabled polarization analysis of off-specular and grazing incidence;
- In-situ ferromagnetic (spin-wave) spectroscopy of thin films ;

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Abstract # 42

CLIC1 interaction with Model Membranes

Sterols have been reported to modulate conformation and hence function of several membrane proteins. One such group is the Chloride Intracellular Ion Channel (CLIC) family of proteins. These largely soluble proteins can spontaneously insert into phospholipid bilayers to form integral membrane ion channels [1]. To date, the structure of their membrane-bound form and factors influencing their auto-insertion remains largely unknown. We have performed Langmuir-film, X-ray, and neutron reflectivity experiments to study the interaction of wild-type or mutant versions of CLIC1 with monolayers prepared with mixtures of different phospholipids and sterol molecules. We investigated the regulatory role of different membrane lipid combinations on the spontaneous membrane insertion of CLICs and elucidated the structural features of the CLIC1 membrane-bound form within these lipid monolayers.

We have shown that CLIC1, in cholesterol containing lipid monolayers, showed significant interaction into the acyl chain region, whereas when cholesterol was absent insertion was limited to the head-group region only. CLIC1 membrane insertion, a pre-cursor to forming functional ion channels is therefore cholesterol dependent [2].

We have also demonstrated for the first time that the GXXXG motif in CLIC1 acts as the cholesterol-binding site for the initial recognition and binding to membrane cholesterol [3]. Further experiments with a variety of sterols confirmed that the interaction between CLIC1 and sterols is dependent on an intact 3β-OH group in the sterol ring. Modification of the sterol structure by the introduction of additional hydroxyl groups and methylation of the sterol alkyl chain was shown to increase membrane insertion of the protein within the phospholipid monolayer [4]. These findings provide clear evidence for the important role of sterols in the regulation of CLIC1 membrane interactions and a putative mechanism for its initial binding and membrane integration.

References

[1]. Valenzuela, S., et al., Regulation of the membrane insertion and conductance activity of the metamorphic chloride intracellular channel protein CLIC1 by cholesterol. PLoS One., 2013. 8(2).
[2]. Hossain, K.R., et al., X-ray and Neutron Reflectivity Study Shows That CLIC1 Undergoes Cholesterol-Dependent Structural Reorganization in Lipid Monolayers. Langmuir, 2017. 33(43): p. 12497-12509.
[3]. Hossain, K., et al., A conserved GXXXG motif in the transmembrane domain of CLIC proteins is essential for their cholesterol-dependant membrane interaction. Biochim Biophys Acta Gen Subj., 2019. 1863(8): p. 1243-1253.
[4]. Hossain, K., et al., Sterol Structural Features' Impact on the Spontaneous Membrane Insertion of CLIC1 into Artificial Lipid Membranes. Langmuir., 2023. 39(9): p. 3286-3300.

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Abstract # 43

Upgrades to the Kowari Strain Scanner

This poster will highlight some recent upgrades to the Kowari slit system including full motorisation of the primary slits and upgrades to the secondary slits. Of focus though, will be the plan to integrate an Aramis image correlation camera on the instrument to work in conjunction with the SScans virtual instrument software as well as the ATOS-5 structured light scanner. These upgrades when implemented will allow instant positioning of samples on the stage with respect to the beam WITHOUT the need for entering curves for positioning!

Authors: **Dr REID, Mark (ANSTO)**, QIU, Zhijun

Abstract # 44

Neutron reflectometry for in operando characterisation of the solid electrolyte interphase (SEI) in electrochemical lithium-mediated nitrogen reduction reactions (Li-NRR)

As the global population grows, the demand for essential resources such as food and energy will place a significant strain on the climate owing to the high levels of anthropogenic emissions generated during production. Despite advancements in renewable energy sources, such as solar power, the limitations of existing infrastructure hinder our ability to efficiently distribute harvested energy. Converting energy into chemical fuels allows for reliable long-term storage, enabling locally harvested renewable energy solutions to be utilised worldwide. Carbon-free options, such as ammonia, can be engineered to ensure negligible emissions at the point of use[1,2]. To produce economically viable, truly carbon-free ammonia fuel, it is essential to develop an energy-efficient synthesis process.

An ammonia synthesis method growing in popularity is the electrochemical reduction of nitrogen from the atmosphere. Whilst protons would ideally be obtained from a sustainable resource such as the electrolysis of water, the delivery of protons must be precisely controlled due to direct competition from the hydrogen evolution reaction (HER)[3,4]. To date, strictly aprotic, lithium mediated systems are the only systems that exhibit performance relevant to the industrial scale[5,6]. Further improvements are still required (alternative mediators[7,8], electrolyte decomposition[9,10] proton donors[10]) to enhance the sustainability of this technology. Accurate assessment of these changes will require comprehensive investigation of the solid electrolyte interface (SEI).

This research, conducted at ANSTO's Open Pool Australian Light-water Reactor (OPAL), focuses on the development of high-performance electrochemical cells optimised for in operando analysis using neutron reflectometry. This approach allows for characterisation of the SEI layer composition across various mediators, electrolytes, and proton delivery systems. The advanced procedures and analysis techniques developed by this work will be discussed. Importantly, this methodology constitutes a versatile and comprehensive ongoing research project, which will continuously be adapted to accommodate future advancements in electrochemical Li-NRR system development.

References

[1]. W. I. F. David et al., 2023 roadmap on ammonia as a carbon-free fuel. Journal of Physics: Energy 6, 021501 (2024).
[2]. D. R. MacFarlane et al., A Roadmap to the Ammonia Economy. Joule 4, 1186-1205 (2020).
[3]. B. H. R. Suryanto et al., Nitrogen reduction to ammonia at high efficiency and rates based on a phosphonium proton shuttle. Science 372, 1187-1191 (2021).
[4]. N. Lazouski, M. Chung, K. Williams, M. L. Gala, K. Manthiram, Non-aqueous gas diffusion electrodes for rapid ammonia synthesis from nitrogen and water-splitting-derived hydrogen. Nature Catalysis 3, 463-469 (2020).
[5]. S. Li et al., Long-term continuous ammonia electrosynthesis. Nature 629, 92–97 (2024).
[6]. H.-L. Du et al., Electroreduction of nitrogen with almost 100% current-to-ammonia efficiency. Nature 609, 722-727 (2022).
[7]. X. Fu et al., Calcium-mediated nitrogen reduction for electrochemical ammonia synthesis. Nature Materials 23, 101-107 (2024).

[8]. M. Krebsz et al., Reduction of dinitrogen to ammonium through a magnesium-based electrochemical process at close-to-ambient temperature. Energy & Environmental Science, (2024).
[9]. A. N. Dey, E. J. Rudd, Electroinitiated Polymerization of Tetrahydrofuran. Journal of The Electrochemical Society 121, 1294 (1974).
[10]. N.-T. Nguyen et al., Nitrogen electroreduction to ammonia with phosphonium proton shuttles: Mass-transport vs. electrode surface chemistry effects. Chem, (2024).

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Abstract # 45

Polarised Neutron Scattering Capabilities at ACNS

The ability to select and manipulate the spin of neutrons as part of scattering experiments enables unique information to be obtained for a variety of samples, ranging from detailed studies of magnetic ordering to the separation of coherent and incoherent scattering which can be especially useful for samples containing a significant amount of hydrogen. This poster will provide an overview of the polarised neutron scattering capabilities which are available for user experiments at ACNS, as well as some information about important considerations when planning a polarised neutron experiment. Details will also be shared about some new technical development projects which aim to improve these offerings, such as a new magnetic guide field system for triple axis spectrometers, and a new laser optical pumping system which is currently under commissioning.

Author: MANNING, Andrew (ANSTO)

Abstract # 46

Recent polarised neutron experiments at ACNS

In this presentation, several recent experiments using polarised neutrons at ACNS will be described. One experiment used polarisation analysis on the cold triple-axis spectrometer Sika to complement a previous unpolarised measurement of a polyelectrolyte sample on the backscattering spectrometer Emu in the quasi-elastic neutron scattering (QENS) regime. This allowed the Kohlrausch-Williams-Watt stretched exponential function describing polymer relaxation in the dynamic structure factor of the sample, which we identified as the incoherent scattering component, to be unambiguously separated from the remaining coherent scattering contribution. This study also compared the relative performance of a diffraction-mode measurement which integrates over all energies to an elastic-mode measurement which accepted a much narrower neutron energy range at the detector, to determine which approach would yield better results.

Another experiment required a strong magnetic field to be applied in the scattering plane for a polarised study of a chiral magnet structure on the thermal triple-axis spectrometer Taipan. This presented several technical challenges in terms of both designing a device to apply such a field over the necessary range of scattering angles, as well as preventing the polarised 3He spin filters from being depolarised by stray magnetic fields on a time scale too short to perform a measurement. The successful implementation of this setup enabled the reversal of magnon spin currents at a critical temperature in a ferrimagnetic terbium garnet to be observed, which can be understood as a manifestation of the spin-Seebeck effect.

Authors: **MANNING, Andrew (ANSTO);** RULE, Kirrily (ANSTO); DE SOUZA, Nicolas (ANSTO - Australian Centre for Neutron Scattering); YANO, Shinichiro (NSRRC)

Abstract # 48

Cultural Heritage research using neutron methods at ACNS

A major challenge in the investigation of material documents of cultural, historical and archaeological significance is the need of non-invasive scientific analytical methods to better understand our past thought the characterisation of ancient artefacts while preserving their unique value and integrity for transmission to future generations. This challenge is particularly evident in the study of ancient metals. Although laboratory-based techniques can provide valuable information, in some cases these conventional methods present strong limitation in terms of penetration depth and representativeness.

Neutron methods have emerged as a highly sensitive, accurate and non-invasive tool for archaeometallurgy investigations. The fundamental properties of the neutron — no electric charge, deep penetration power into matter, and interaction with the nucleus of an atom rather than with the diffuse electron cloud —make this sub-atomic particle the ideal probe to survey the bulk of dense materials like metals.

In this paper a selection of relevant cross-disciplinary studies conducted at the Australian Nuclear Science and Technology Organisation (ANSTO) and undertaken in collaboration with Australian and international stakeholders will be showcased: from the advanced manufacture of arms and armours to the secret of votive items, through the invention of coinage.

Author: SALVEMINI, Filomena (ACNS-ANSTO)

Abstract # 49

Study Multiferroic/Magnetoelectric Materials using Inelastic Neutron Scattering Technique

Multiferroic and magnetoelectric materials have been extensively studied in the past two decades due to their interesting properties and potential versatile applications. Magnetoelectric coupling is the fundamental mechanism of multiferroic and magnetoelectric properties in these materials. However, understanding magnetoelectric coupling mechanisms in these materials is a challenging task. Magnetoelectric coupling mechanisms are highly dependent on magnetic structures and spin dynamics. Neutron diffraction and inelastic neutron scattering are powerful tools to study these materials to reveal their hidden magnetoelectric coupling mechanism. Spin dynamics of multiferroic/magnetoelectric materials such as TbMnO3[1], BiFeO3[2], Co4Nb2O9[3,4]/Mn4Nb2O9[5] have been intensively investigated using the inelastic neutron scattering technique. The results from these studies significantly improve our understanding to the magnetoelectric coupling mechanism in these complicated multiferroic systems. All these studies evidence that inelastic neutron scattering technique is an indispensable tool to study the microscopic mechanism of magnetoelectric coupling in various multiferroic/magnetoelectric systems. The thermal-neutron triple-axis spectrometer Taipan[6] and the cold-neutron triple-axis spectrometer Sika[7] at Australian Centre for Neutron Scattering (ACNS) are powerful tools to conduct inelastic neutron scattering studies of condensed matters including multiferroic materials.

Reference

[1] M. Kenzelmann, A. B. Harris, S. Jonas, C. Broholm, J. Schefer, S. B. Kim, C. L. Zhang, S.-W. Cheong, O. P. Vajk, and J. W. Lynn, Phys. Rev. Lett. 95, 087206 (2005)
[2] Jaehong Jeong, E. A. Goremychkin, T. Guidi, K. Nakajima, Gun Sang Jeon, Shin-Ae Kim, S. Furukawa,Yong Baek Kim, Seongsu Lee, V. Kiryukhin, S-W. Cheong, and Je-Geun Park, Phys. Rev. Lett. 108, 077202 (2012)
[3] G. Deng, Y. Cao, W. Ren, S. Cao, A. Studer, N. Gauthier, M. Kenzelmann, G. Davison, K. Rule, J. S. Gardner, P. Imperia, C. Ulrich, and G. J. McIntyre, Phys. Rev. B 97, 085154 (2018)
[4] G. Deng, Y. Yu, Y. Cao, Z. Feng, W. Ren, S. Cao, A. J. Studer, J. R. Hester, Y. Kareri, C. Ulrich, and G. J. McIntyre, J. Phys.: Condens. Matter 31, 235801 (2019)
[5] G. Deng, G. Zhao, S. Zhu, Z. Feng, W. Ren, S. Cao, A. Studer, and G. J. McIntyre, New J Phys. 24, 083007(2022)
[6] S. A. Danilkin and M. Yethiraj, Neutron News 20, 37 (2009)
[7] C-M Wu, G Deng, J Gardner, P Vorderwisch, W-H Li, S Yano, J-C Peng and E, Imamovic, J. Instrum. 11 P10009 (2016)

Authors: **DENG, Guochu (ANSTO);** MCINTYRE, Garry (ANSTO)

Abstract # 50

Methods to calculate the corresponding neutron scattering length density from spin-polarised density functional theory

Spin polarised density functional theory can predict the magnetic moment and arrangement of spins in a crystal structure from ab initio calculations. We will present DFT calculations on transition metal doped SnTe, predicting the size of the magnetic moment for Fe,Cr, V, Ti dopants.

Once the size and spatial distribution of the magnetic moments is known from DFT, it is straightforward to calculate the neutron scattering length density, which is the measurable in polarised neutron reflectometry experiments. To achieve this, we will present a simple Python-based procedure that converts the output files from Quantum Expresso and VASP into the corresponding neutron scattering length density.

Authors: **Mrs SHABBIR, Syeda Amina; Dr DAVID, Cortie**

Abstract # 51

Pydingo, a new GUI software package for simple CT reconstruction

The neutron imaging instrument DINGO did use Octopus for CT reconstruction since operational until Ocotpus has withdrawn further support. We tried several new software packages and did end up using Tomopy and the graphical extension Neutompy for a while. Unfortunately, these packages require some skills in python scripting and lacking user friendliness. Because of our diverse customer base, we were looking into a user-friendly GUI providing the functionality of Tomopy and the GPU acceleration of the Astra Toolbox. A new MacOS version without GPU acceleration is available as well.

The new developed Pydingo provides once installed easy access to Tomopy and the Astra Toolbox through its GUI which comes in three different sections. The first section handles the repreparation of the raw data including normalisation and selection of region of interest. A new algorithm for intensity correction and beam hardening is included. In addition, a phase retrieval can be selected. The corrected image output will be handled in a second section calculating the centre of rotation, tilt and final reconstructed slices. The reconstruction algorithm is available for parallel and cone beam geometry. All GUIs are open source and can be extended with additional correction and reconstruction algorithms.

Authors: **GARBE, Ulf (ANSTO);** Dr PILLICCIA, Daniele (IDtools)

Abstract # 52

Small-Angle Neutron Scattering Analysis of a Novel Microemulsion-Based Electrolyte

In this study, we introduce a novel class of aqueous electrolytes based on microemulsions that demonstrate an impressive high voltage window (2.2–2.5 V) and outstanding performance in supercapacitors. The electrochemical behavior is strongly influenced by the electrode morphology, specific surface area, and electrolyte composition. The extended voltage window is linked to the formation of a hydrophobic lamellar region aligned perpendicular to the electrode surface, followed by a bulk conductive microemulsion phase. Small-angle neutron scattering (SANS) analysis revealed a structural transition from normal ellipsoids to bicontinuous systems as the water-to-oil ratio in the bulk conductive phase increases. Additionally, the analysis showed that these phases remain stable across a wide temperature range, with only a slight reduction in domain size for the bicontinuous phase and droplet sizes of the ellipsoids. This innovative microemulsion-based aqueous electrolyte offers a promising pathway for designing high-voltage aqueous electrolytes, unlocking the safety and cost advantages of aqueous systems.

Authors: **SALISU, Aliyu (University of Newcastle);** MATA, Jitendra (ANSTO); HOLT, Stephen (ANSTO); PETERSON, Vanessa (ANSTO); Dr V GOREHAM, Renee (University of Newcastle); Prof. NANN, Thomas (Allegro Energy)

Abstract # 53

Update from the Australian Centre for Neutron Scattering

The Australian Centre for Neutron Scattering (ACNS) utilises neutrons from Australia's multi-purpose research reactor, OPAL, to solve complex research and industrial problems for Australian and international users via merit-based access and user-pays programs. The neutron beam facilities of OPAL consist of neutron beam tubes that penetrate the reflector vessel, a cold neutron source, beam shutters and neutron guides. A suite of 15 neutron beams instruments utilise both the thermal and cold neutron beams for both atomic and molecular structure determination and dynamics measurements, residual stress measurement and neutron imaging. An update will be given on the OPAL reactor and its neutron beam facilities, recent upgrades, user program, and future plans.

Author: **SCHULZ, Jamie (ANSTO)**

Abstract # 54

Additive Friction Stir Deposition (AFSD) for High-Strength Aluminium Alloys

Additive Friction Stir Deposition (AFSD) is a rapidly emerging solid-state additive manufacturing (AM) process characterised by high deposition rate. As a non-fusion AM technique, AFSD avoids defects related to melting, such as solidification cracking, allowing for the processing of high-strength aluminium alloys with solidification cracking susceptibility. Additionally, AFSD generates lower residual stress compared to other AM processes. The severe plastic deformation inherent in the process promotes metallurgical bonding between dissimilar aluminium alloys and facilitates the breakup of brittle intermetallics, making AFSD suited for utilising recycled feedstock material. However, the thermal cycling during layer deposition affects the precipitation-strengthening mechanism in high-strength aluminium alloys, leading to hardness gradient in as-manufactured structure.

This study investigates the microstructure and defect formation in a two-step AFSD-manufactured Al6061 structure with deposit heights of 18.5 mm and 10.5 mm. Residual stress analysis is performed on a three-step Al6061 structure with deposit heights of 9.5 mm, 6.5 mm, and 3.5 mm. Additionally, we present preliminary results on the microstructure, material distribution, hardness, and residual stress of a 4 mm-high recycled aluminium structure manufactured via AFSD using alternating Al6061/Al7075 feedstock.

The microstructure is characterised using optical microscopy, scanning electron microscopy, energy-dispersive X-ray spectroscopy, and electron backscatter diffraction, while material flow and defect analysis is performed via X-ray computed tomography. Hardness mapping is employed to assess the mechanical properties, and residual stress distribution is measured non-destructively using neutron diffraction. The findings from this research provide critical insights for the large-scale industrial application of AFSD.

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Abstract # 55

Neutron Imaging for Palaeontology

Palaeontology and evolutionary studies are dependent on the physical measurement of bone dimensions to determine relationships between organisms, determine age at death, interpret lifestyles, predator-prey interactions and physical adaptions to a constantly changing world. These measurements have traditionally demanded the physical extraction of specimens from their surrounding rock. This process risks damage to small and fragile bones, loss of contextual information associated with the environment at that time, mode of preservation and articulation. For this reason, 3D imaging using X-rays has become a critical tool for the investigation and preservation of fossilised remains, which can now be investigated while remaining in their original matrix. For many fossil localities, the applicability of X-rays is limited due to the prevalence of authigenic pyrite - pyrite that forms within, and surrounding fossils due to the localised reduction of sulfate (from decomposing organic remains) in iron-rich pore waters. These iron-rich minerals are opaque to X-rays, and therefore obscure the fossil remains.

Neutron imaging is a relatively new tool for palaeontology and has revolutionised the field for two reasons: a high-sensitivity to hydrogen, and greater ability to penetrate through iron-rich minerals such as pyrite.

This presentation draws on high-profile palaeontological studies conducted using the DINGO neutron imaging instrument at ANSTO to demonstrate the complementarity of neutrons with X-rays. The method has become a game-changer for Australian palaeontology, attracting specimens for study from around the globe. It will highlight the advantage of neutrons in revealing cartilaginous soft-tissue remains, complete internal organs, stomach contents and entire organisms that are invisible to traditional X-ray tomography.

Author: **BEVITT, Joseph (ANSTO)**

Abstract # 56

Deuterium labelling at the National Deuteration Facility: facility overview, capability advancements and impact

The use of deuterated molecules in neutron scattering experiments for investigating the relation- ship between molecular structure and function expands the range and complexity of science that can be conducted at reactor and spallation-source neutron facilities. There have been increasing global demand and initiatives in the field of molecular deuteration in the recent years; however, the complexity of the required molecules for new experiments has also increased. This has limited the experiments that can be performed and formed a bottle-neck for advancing the applications of neutron scattering. In this presentation, recent capability advancements will be discussed and the impact of deuteration on the research outcomes achieved by using bespoke deuterated molecules produced by the National Deuteration Facility (NDF). The NDF has the specialised expertise and infrastructure to provide deuteration through both biological and chemical molecular deuteration techniques for a diversity of molecules. Recent high impact case studies will be presented which reveal the exciting and diverse characterisation studies which are now available for the neutron research community, describing the synthesis and application of deuterated molecules which are unavailable from commercial sources.

Author: DARWISH, Tamim (ANSTO)

Abstract # 57

Recent developments on Echidna

Echidna has just installed an improved monochromator, providing both increased intensity for common wavelengths and convenient access to a new wavelength, 2.05Å at the standard 140° takeoff angle. The new monochromator is characterised in this poster, together with insights into Echidna usage and exploration of performance limits, including: how little sample is needed? What is the detection limit for magnetic moments? How absorbing can my sample be?

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